Amendments to the Specification

Please replace the first paragraph on page 26 of the specification with the following paragraph:

Dipolar couplings were calculated as the difference between the oriented couplings ($^1J_{CH}$ + D_{CH}) and the isotropic couplings ($^1J_{CH}$). In each case, couplings were extracted using a Bayesian time-domain NMR parameter estimation program Xrambo, using the method described (5). This program is available on the Internet at ~~http://tesla.ccrc.uga.edu~~ http://tesla.ccrc.uga.edu. Typically, a 2D HSQC data set with the desired splittings in the direct dimensions was transformed and phased to yield a 1024 x 256 real matrix. Single FID slices across the width of the resonance under investigation were analyzed independently. For every slice, the resulting frequency domain data were reverse Fourier transformed to generate a 1D time domain data set as input for Xrambo. The following model was used for the data. Each component of the doublet resulting from C-H couplings was given an identical linewidth and intensity, but an independent phase to circumvent any problems resulting from the presence of phase twist anomalies or dispersive contributions. Values for shifts, linewidths, phases and intensities were estimated and entered as starting parameters which were subsequently refined by Xrambo's Metropolis Monte Carlo method. This procedure was repeated for several indirect slices of the same doublet and the resulting rmsd across various slices was used as the uncertainty in measurement. The error analysis from this procedure was used to estimate the final precision of all measured residual dipolar couplings. The measured residual dipolar couplings and associated uncertainties along with AMM input coordinates obtained from an MD simulation were then used as input to a singular value decomposition program for the determination of order tensor elements. (6) This program is also available on the internet at ~~http://tesla.ccrc.uga.edu~~ http://tesla.ccrc.uga.edu.